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## Spin-orbit interaction of electrons on curved surface

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**Abstract.** Spin-orbit (SO) interaction of electrons confined near the curved semiconductor surface is studied. The curvature of surface determines the new mechanism of SO interaction which complements the known mechanisms occurring in planar systems. The specific cases of nanosphere and nanotube are considered.

### Introduction

It is well known that the Hamiltonian for electrons, confined near the oriented two-dimensional system, contains linear in lateral momentum  $\mathbf{p}$  terms, which describe the spin-orbit (SO) interaction [1]. The orientation of the surface may be determined by the asymmetry of the confining potential [1] as well as by the lack of the inversion symmetry of the initial crystal [2, 3] or the asymmetric orientation of the surface relative to the crystal axes of symmetry.

In the first case (the Rashba model) the SO Hamiltonian has the form [1]:

$$\tilde{\mathcal{H}}_{SO} = \alpha(\hat{\sigma}[\hat{\mathbf{p}} \times \mathbf{n}]), \quad (1)$$

where  $\hat{\sigma}$  are Pauli matrices,  $\hat{\mathbf{p}}$  is the 2D electron momentum. The Hamiltonian (1) appears in the third order on the basic SO interaction. This results in relative smallness of the effective SO interaction for the conduction band electrons in semiconductors with small SO splitting of the valence band edge.

The linear terms in Hamiltonian lead to the spin-splitting of energy bands in the absence of magnetic field and to the possibility of electric-field-induced spin-flip transitions [3]. Recently SO was shown to be responsible for spin ordering by a lateral electric field [4] and a mixed spin-plasmon polaritons [5]. SO interaction of electrons on the cylindrical surface were studied in [6,7] on the basis of the Rashba model.

In the present paper we draw attention to the fact that the curvature itself marks down the surface orientation and hence causes the additional SO interaction. This curvature-induced SO interaction is proportional to the ratio of quantum well width to the radius of curvature. Most distinctly the proposed mechanism can be illustrated by the difference of the planar quantum well and a system with the spherical symmetry. In symmetric planar quantum wells the effective SO interaction is absent for free electrons. Conversely, SO interaction in a spherically symmetric system (e.g., atom) does not vanish after averaging over radial states. This means that a spherical system has additional effective SO interaction due to curvature.

### Spherical quantum well

Let us consider a potential  $U(r)$  confining electrons near some radius  $R$  (spherical quantum well). The width of a well  $d$  is supposed to be much less than  $R$ . The same is assumed

concerning the characteristic size of radial states. In this limit effective SO interaction can be expressed in the form containing only the surface coordinates on the sphere.

For spherically symmetric potential the basic SO interaction has the well known form:

$$\mathcal{H}_{SO} = \alpha \frac{1}{r} \frac{dU(r)}{dr} (\hat{\sigma} \hat{\mathbf{l}}). \quad (2)$$

Here  $\hat{\mathbf{l}}$  is the orbital momentum (we set  $\hbar = 1$ ). The coefficient of spin-orbit coupling  $\alpha$  for free electrons is  $\alpha = 1/4(m_e c)^2$ , where  $m_e$  is the electron mass,  $c$  is the velocity of light. In the two-band Dirac model of semiconductor bands,  $\alpha = 1/2 E_g m_e$ , where  $E_g$  is the width of the forbidden band and  $m_e$  is the effective electron mass.

The Hamiltonian (2) should be averaged over radial states  $\psi_n(r)$  of the Hamiltonian without SO interaction. The radial states satisfy the equation

$$\frac{1}{2m_e r^2} (r^2 \psi_n'(r))' + (E - U(r) - \frac{l(l+1)}{2m_e r^2}) \psi_n(r) = 0, \quad (3)$$

where  $E$  is the energy of the state,  $l$  is the angular momentum.

The averaging should be done by integrating with the measure  $r^2$ . Expressing the result via the radial wave function we have

$$\bar{\mathcal{H}}_{SO} = -\frac{2\alpha}{R} (T_n - T_t) (\hat{\sigma} \hat{\mathbf{l}}) \quad (4)$$

Here

$$T_n = \frac{1}{2m_e} \int (\psi_n'(r))^2 r^2 dr, \quad T_t = \frac{\hat{\mathbf{l}}^2}{2m_e R^2} \quad (5)$$

are the radial and tangential parts of electron kinetic energy, respectively. The integration in (5) is effectively run within the layer of width  $d$  near  $R$  and  $T_n$  has the order of magnitude of  $1/m_e d^2$  for lowest levels.

The Eq. (4) can be rewritten in the other form, using translational momentum  $\hat{\mathbf{p}} = (\hat{p}_\theta, \hat{p}_\varphi) = -i(\partial/\partial\theta, (1/\sin\theta)\partial/\partial\varphi)/R$  on the sphere surface:

$$\bar{\mathcal{H}}_{SO} = \frac{2\alpha}{R^2} (T_n - \frac{\hat{p}^2}{2m_e}) ([\hat{\mathbf{p}} \mathbf{n}_R] \hat{\sigma}) \quad \mathbf{n}_R = \mathbf{R}/R. \quad (6)$$

In the form of Eq. (4) the SO Hamiltonian looks like Rashba Hamiltonian, Eq. (1), for a planar system. Really, in the small neighborhood of some point on sphere the vector  $\mathbf{n}_R$  is constant, the sphere can be considered as a plane, and  $\hat{\mathbf{p}}$  as a usual momentum along the plane. The difference of Eq. (4) and the Rashba Hamiltonian, Eq. (1), lies in the momentum dependence of the SO coupling constant. In particular, it can change sign with the longitudinal energy  $p^2/2m_e$ .

Physically, the SO term, proportional to  $T_n$ , originates from the difference of electron tangential velocity on the inner and the outer well boundaries. In the frame accompanying the rotating electron the electron spin experiences a magnetic field  $\mathbf{B}' = \frac{1}{c} [\mathbf{v} \mathbf{E}]$ , where  $\mathbf{v}$  is the linear velocity of rotation,  $\mathbf{E}$  is a confining electric field of well walls. The averaging of  $\mathbf{B}'$  with respect to radial motion gives a finite result due to angular momentum conservation. The other contribution to SO interaction, proportional to  $T_t$ , originates from magnetic field, induced by the centripetal force. The difference of signs of terms in Eq. (6) is explained by

the difference in directions of dominating accelerations. For specific cases of wells with hard wall potential and a parabolic well ( $U(r) = m_e \omega^2 (r - R)^2 / 2$ ) we have:

$$T_n = \pi^2 n^2 / 2m_e d^2 \quad n \geq 1 \text{ (hard wall);}$$

$$T_n = \omega(n + 1/2)/2 \quad n \geq 0 \text{ (parabolic well).}$$

The change of SO interaction sign occurs at  $p^2/2m_e = \pi^2/2m_e d^2$  and  $p^2/2m_e = \omega/4$ , respectively.

If the number of electrons is small enough, they occupy the bottom of the first radial subband only,  $p^2/2m_e \ll E_2 - E_1$ , and the radial term in Eq. (7) is dominating.

### Cylindrical quantum well

The case of electrons locating on a cylindrical surface can be considered analogously. Starting from the more general expression for SO interaction,  $\mathcal{H}_{SO} = \alpha [\hat{\sigma} \nabla U] \mathbf{p}$  and using cylindrical coordinates  $(\rho, \varphi, z)$  with axis  $z$  directed along the cylinder axis, one can find

$$\mathcal{H}_{SO} = \frac{2\alpha}{R} \left( (\hat{T}_t - T_n) \hat{p}_\varphi \hat{\sigma}_z + \{[\mathbf{n}_\rho \hat{\sigma}]_z, \hat{T}_t\} \hat{p}_z \right), \quad (7)$$

$$T_n = \frac{1}{2m_e} \int (\psi'_n(\rho))^2 \rho d\rho, \quad \hat{T}_t = \frac{\hat{p}_\varphi^2}{2m_e}, \quad (8)$$

where  $\hat{p}_\varphi = -(i/R)\partial/\partial\varphi$ ,  $R$  is the cylinder radius; figure brackets in Eq. (7) stands for the operation of symmetrization:  $\{\hat{A}, \hat{B}\} = (\hat{A}\hat{B} + \hat{B}\hat{A})/2$ .

Note, that the considered SO Hamiltonians contain both the terms, caused by quick transversal motion, depending on the specific structure of transversal wave function, and pure geometrical terms, caused by centripetal acceleration.

The case of slightly curved surface can be studied exploiting the additivity of contributions from the eigenvalues of the curvature tensor. Here we restrict ourselves by the main (transversal) contribution to the SO Hamiltonian, assuming the longitudinal energy to be much less than the distance between the levels of transversal quantization.

Consider the curved surface, tangent to the plane  $(x, y)$  in the point  $0$ , where  $x$  and  $y$  are the main axes of the curvature tensor. The SO Hamiltonian near this point reads as:

$$\mathcal{H}_{SO} = -2\alpha \left( \{ \hat{p}_x, \frac{T_n}{R_x} \} \hat{\sigma}_y - \{ \hat{p}_y, \frac{T_n}{R_y} \} \sigma_x \right), \quad (9)$$

where  $T_n$  is the local transversal kinetic energy (the energy level of the main state of transversal motion),  $R_{x,y}$  are the main curvature radii.

We have also obtained the SO Hamiltonian in the general case of curved surface. Similar to the particular cases of sphere and cylinder this Hamiltonian contains terms due to transversal wave function structure and centripetal acceleration. This Hamiltonian can be used to find the energy states on the curved surface without and with external fields. It is also useful for calculation of responses to external fields.

Generally speaking, the obtained curvature-induced SO Hamiltonians should be added by the other (mentioned in the Introduction) terms, which are not related with the curvature. In dependence on the radius of curvature one or another mechanism will prevail. For lesser radii the curvature contribution becomes more essential.

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